Computing Sciences
Atomic and Molecular Theory Group

Interaction Between Virtual States and Resonance States in Electron-Polyatomic Collisions

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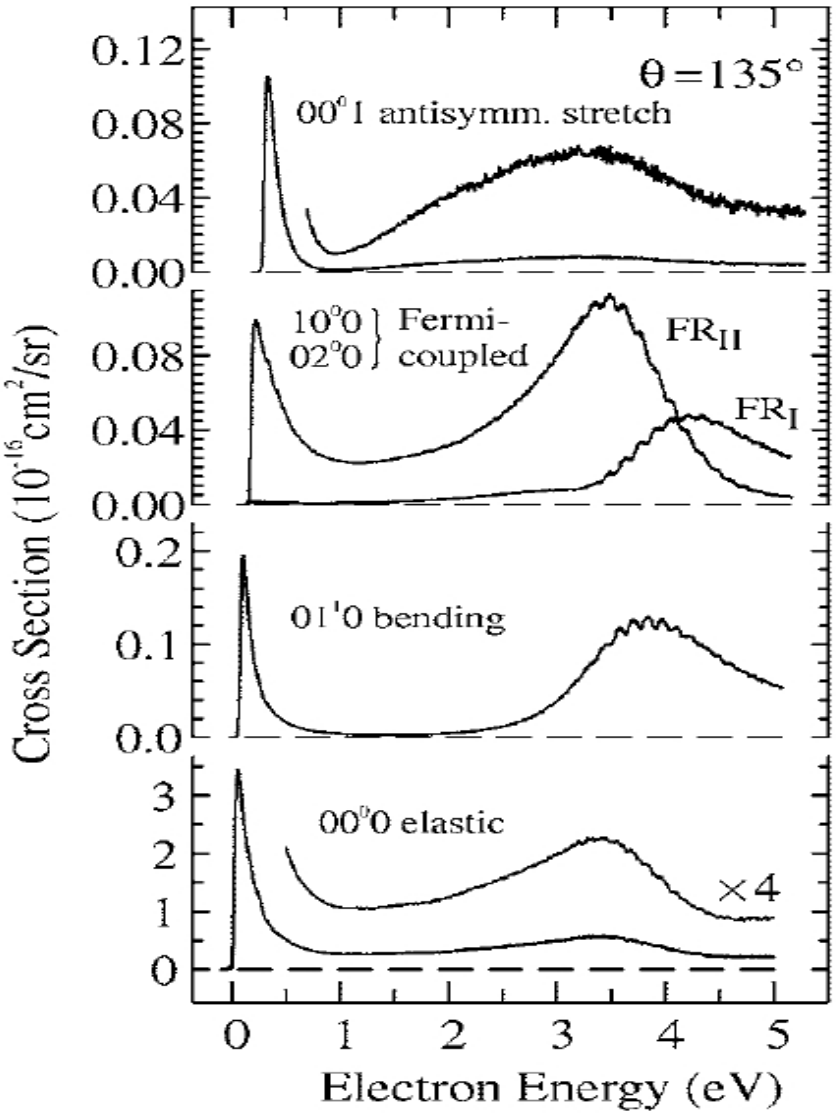

Figure 1: High precision electron-$C0_2$ scattering experiment by Allan J. Phys B **35** L387 (2002)

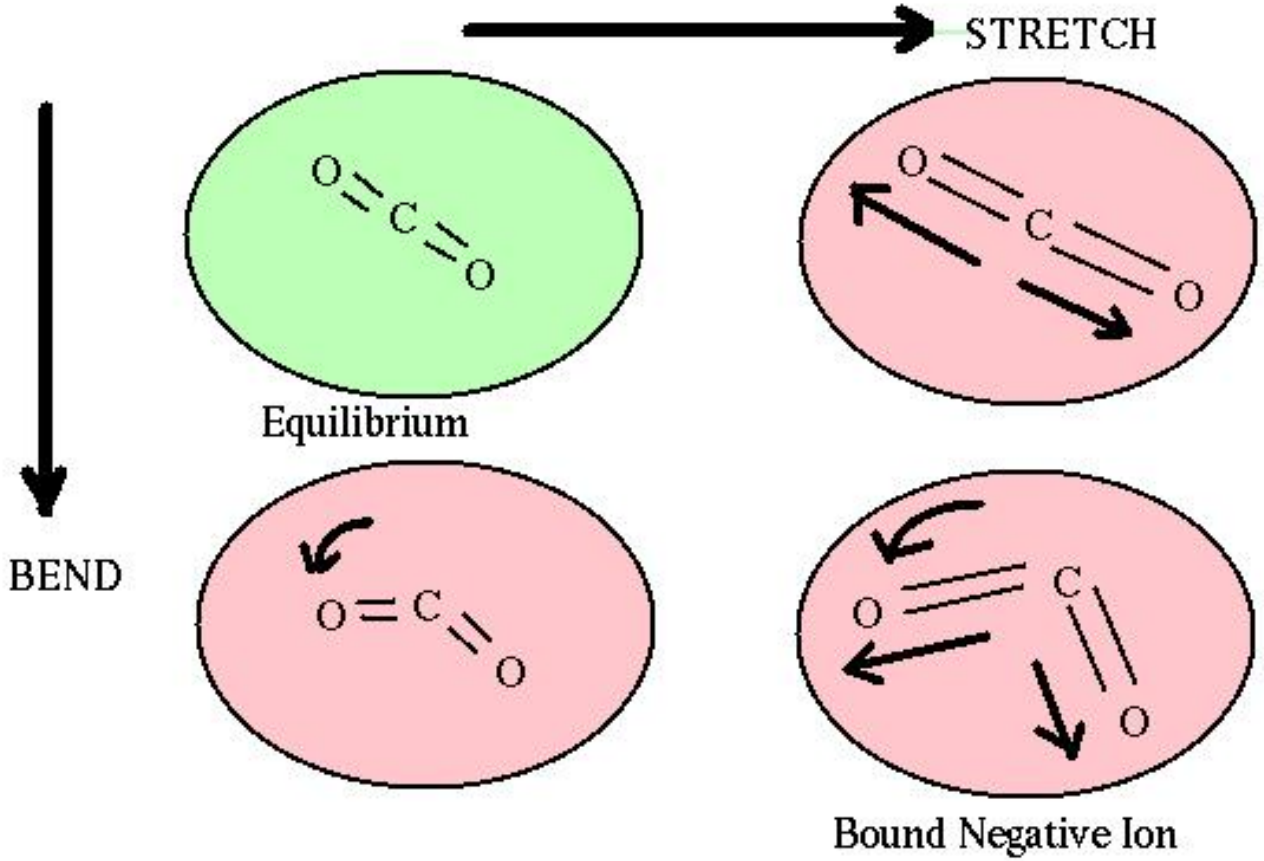

Figure 2: cartoon of different configurations of CO_2^-

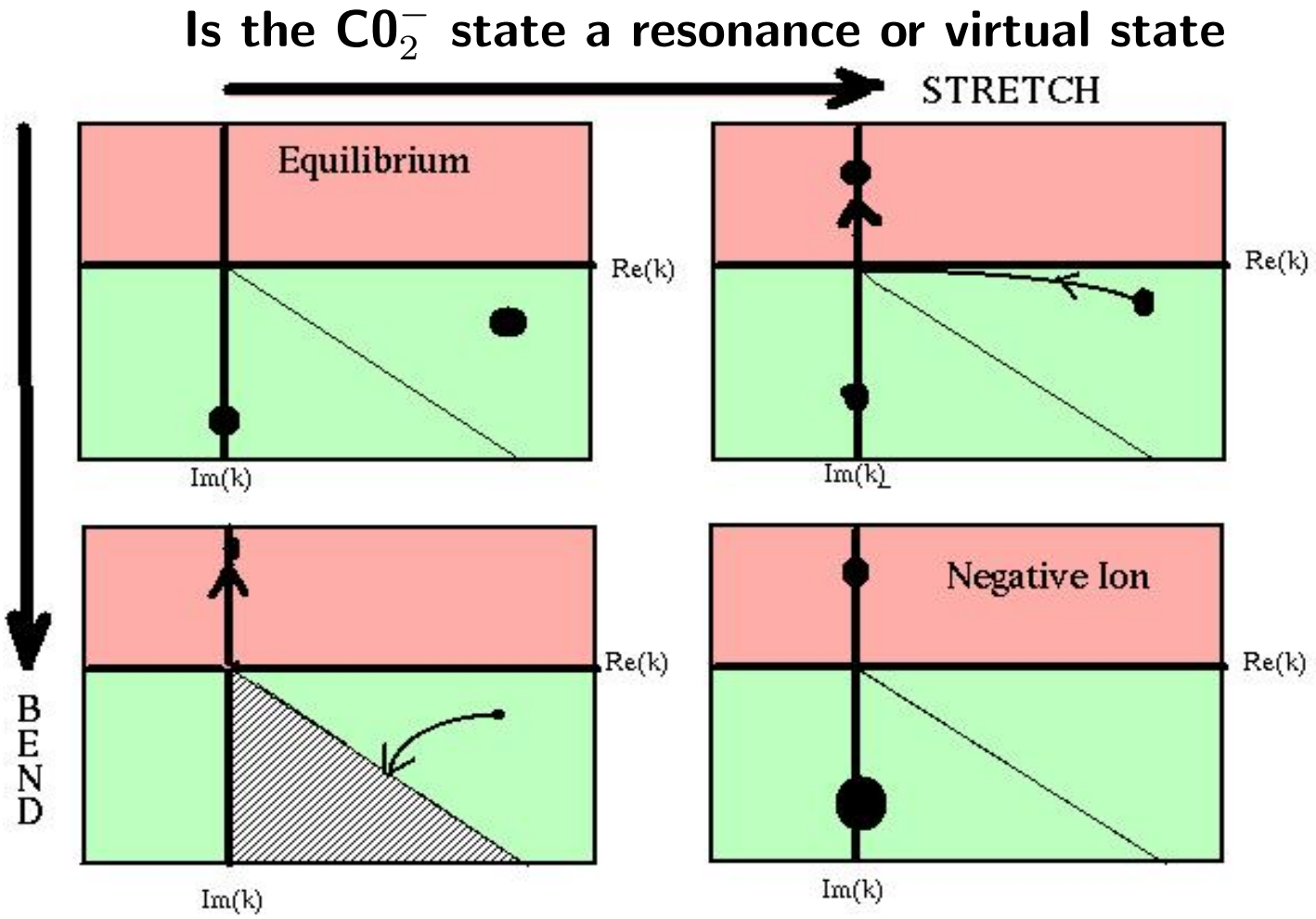

Figure 3: Interpretation of fixed-body calculations by Rescigno $et\ al$ in the complex k-plane (Phys Rev A **65** 032716 (2002))

Dipole potential couples all partial waves

$$\left(T + V_{l,l'}(r) - E\right) \psi_{l'}(r) = 0 \tag{1}$$

$$V_{l,l'}(r \to \infty) = \text{multipole terms} \tag{2}$$

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$$\begin{pmatrix} -\frac{1}{2}\frac{d^2}{dr^2} + V_0(r) - \frac{k^2}{2} & C(r) \\ C(r) & -\frac{1}{2}\frac{d^2}{dr^2} + V_1(r) - \frac{k^2}{2} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = 0 \tag{3}$$

where

$$V_0(r \to \infty) = 0 \tag{4}$$

$$V_1(r \to \infty) = \frac{l(l+1)}{2r^2} \tag{5}$$

$$C(r \to \infty) = \frac{d}{r^2} \tag{6}$$

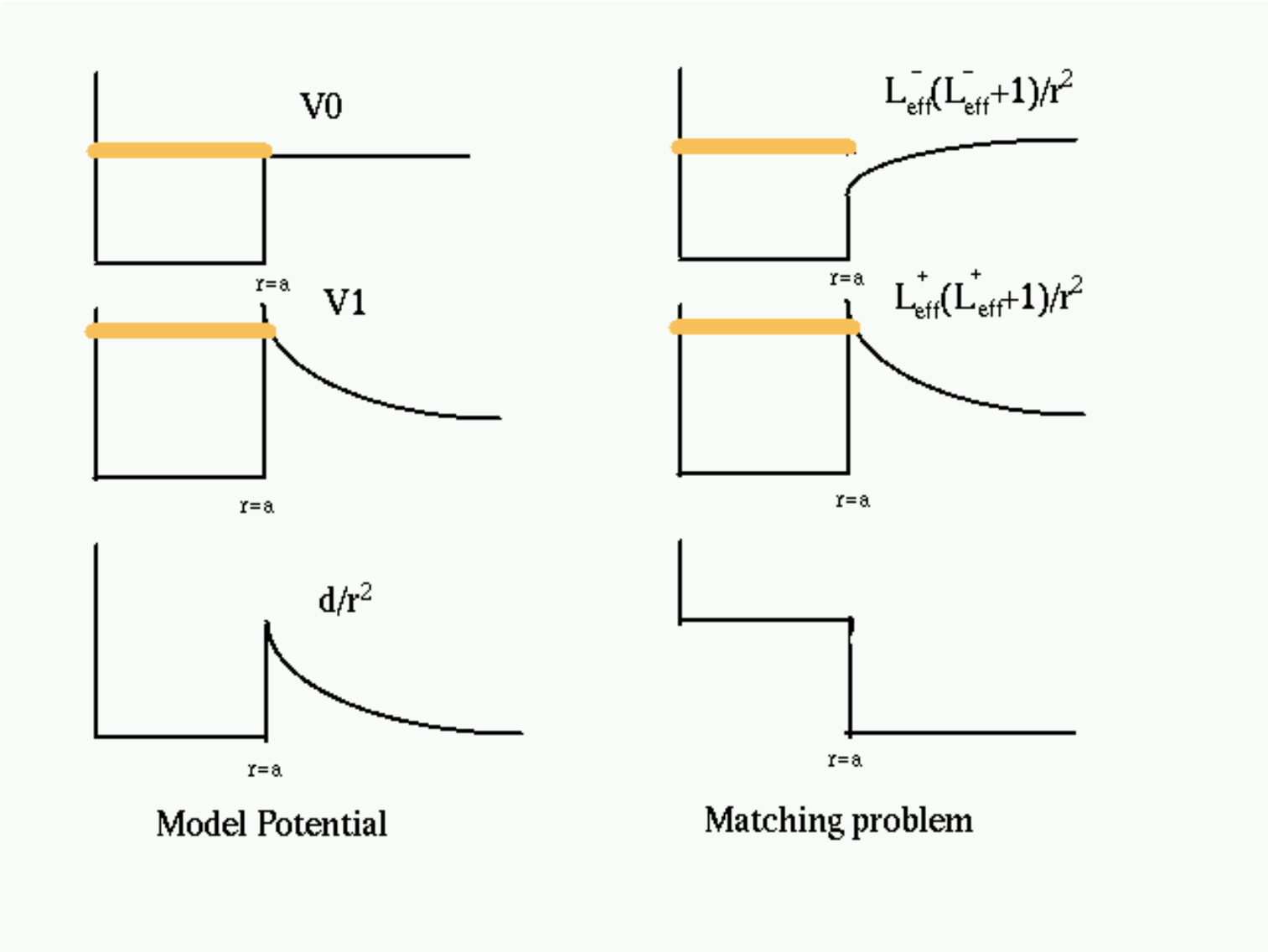


Figure 4: Model for the potentials. Leads to an analytic expression for the S-matrix

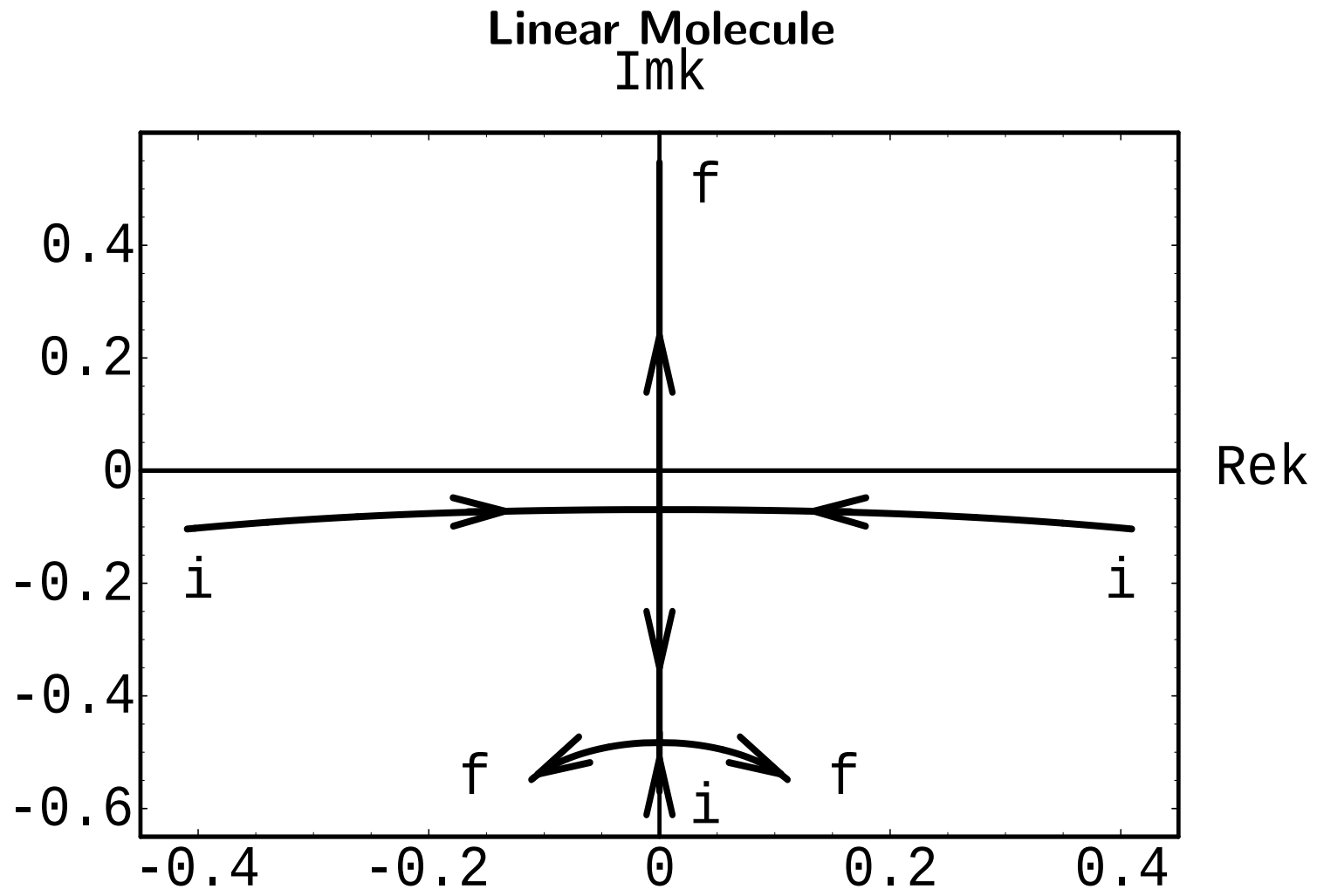


Figure 5: Trajectories of the S-matrix poles as we stretch the molecule

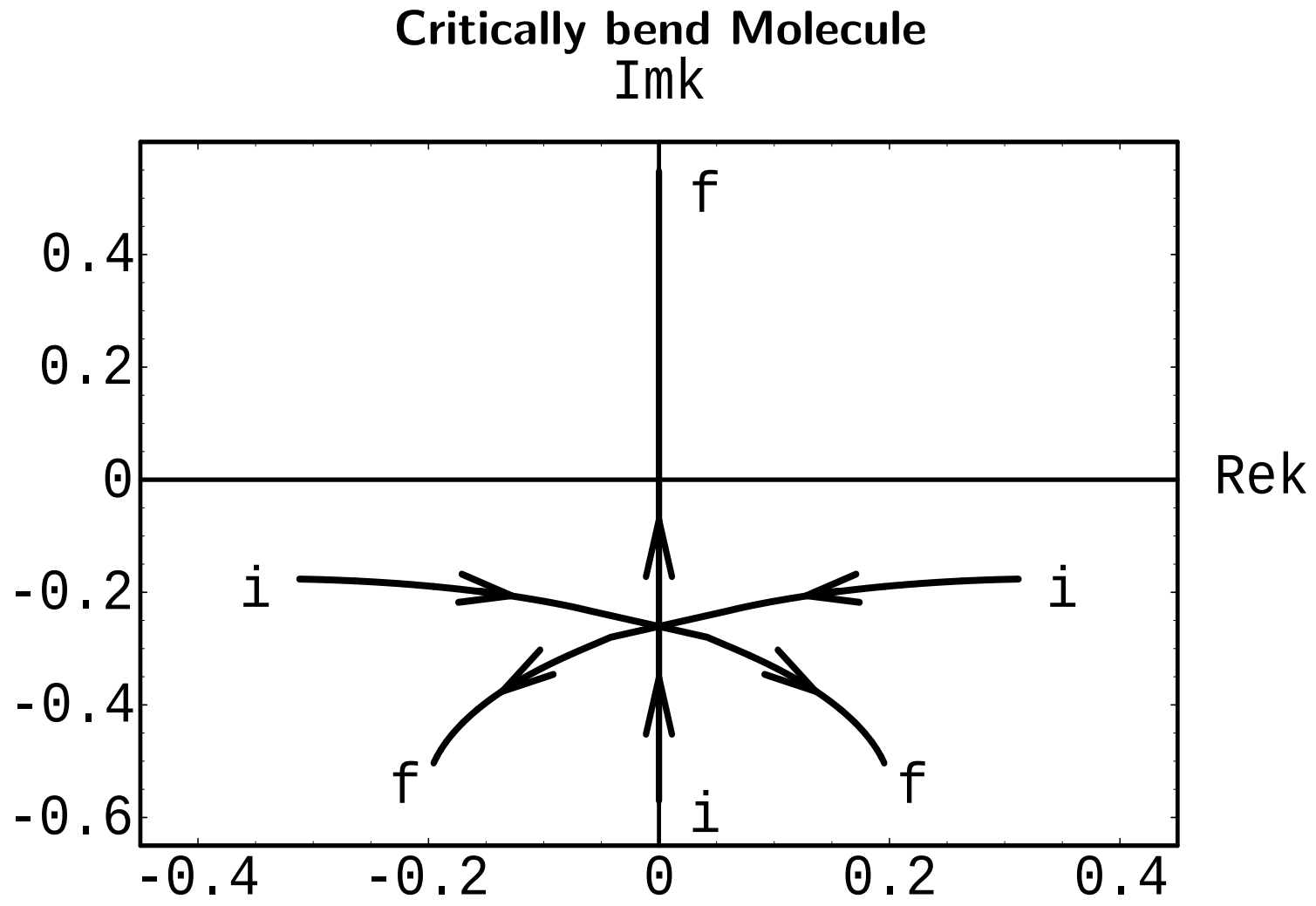


Figure 6: Trajectories of the S-matrix poles as we stretch the molecule

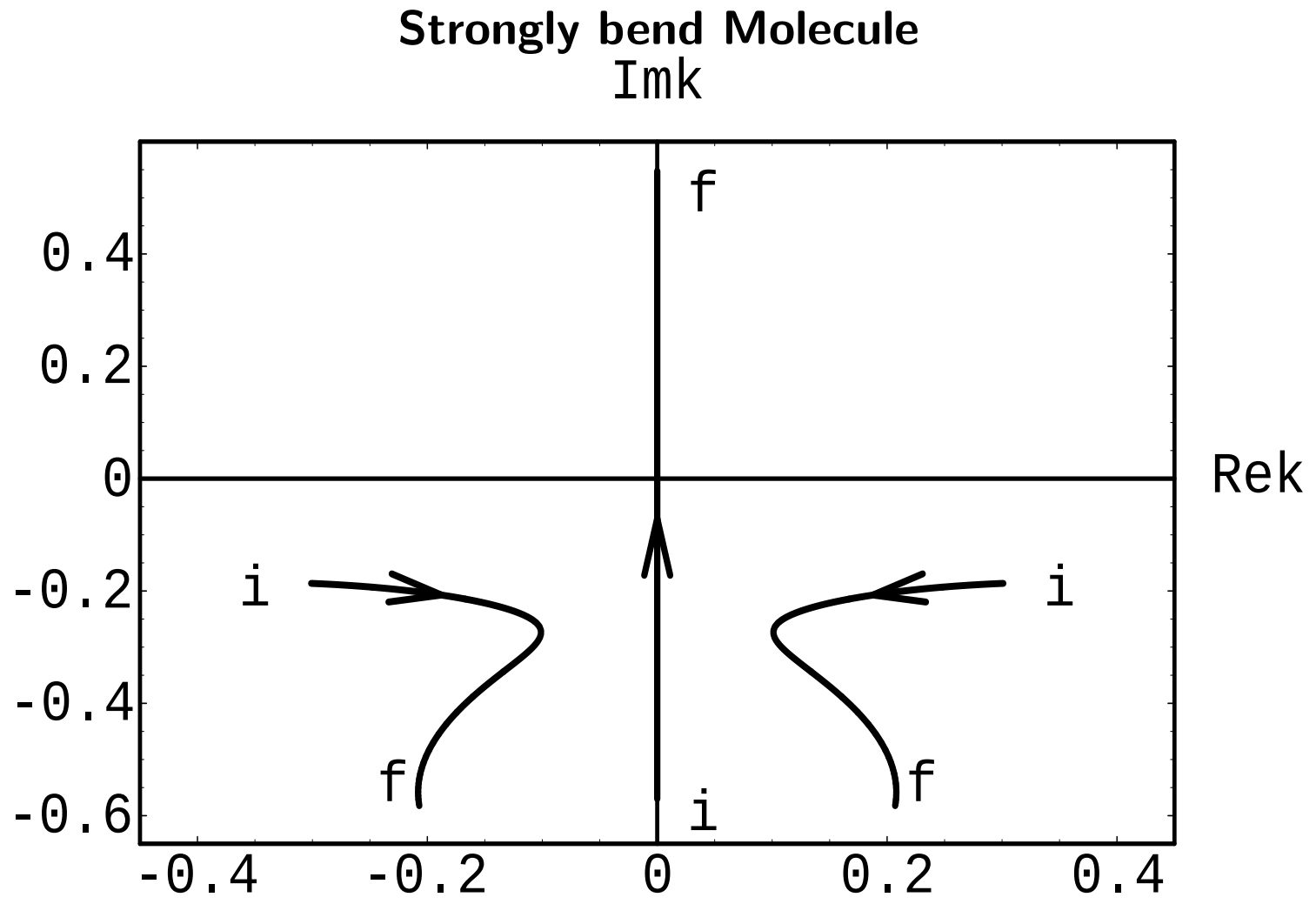
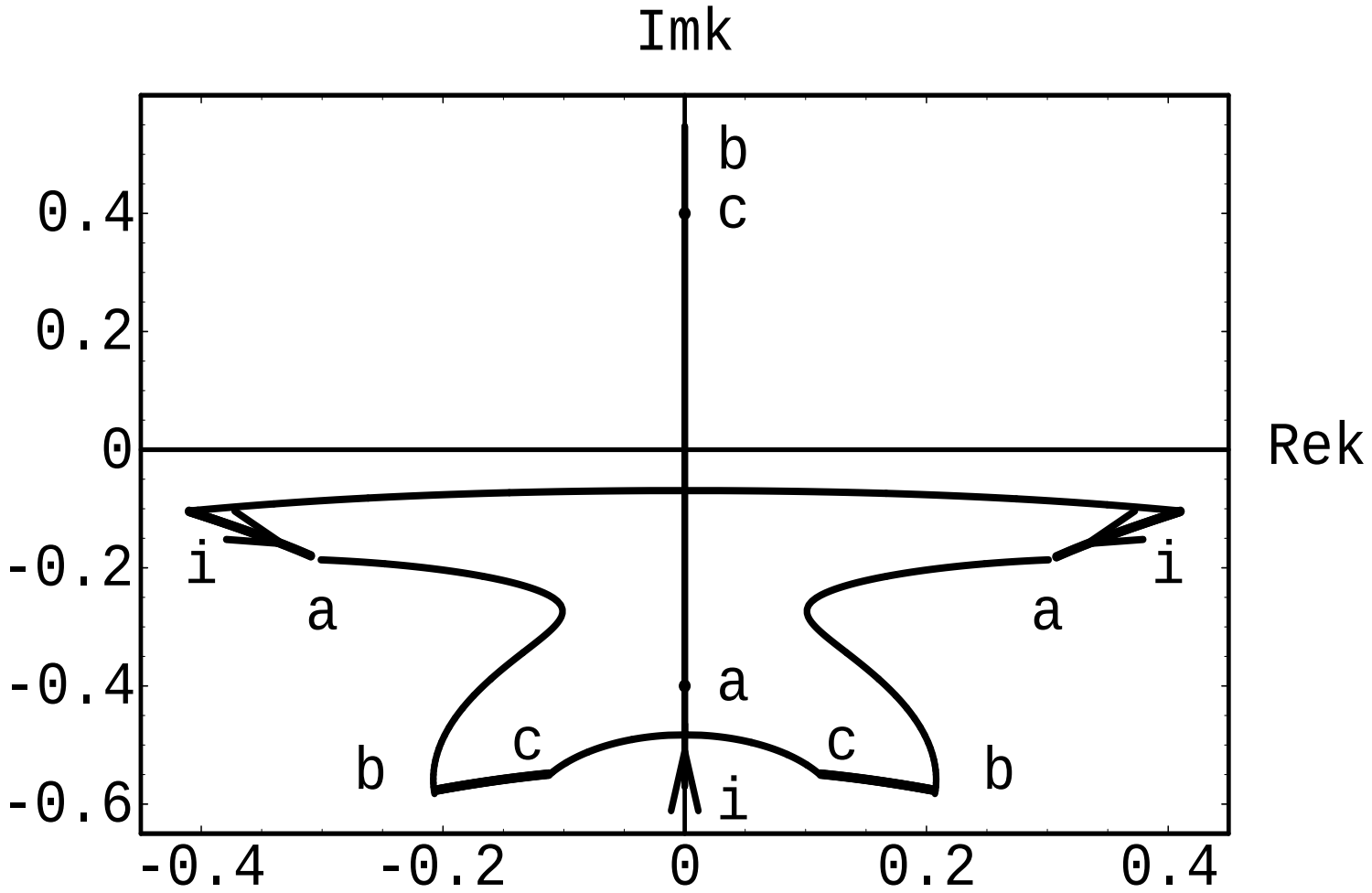
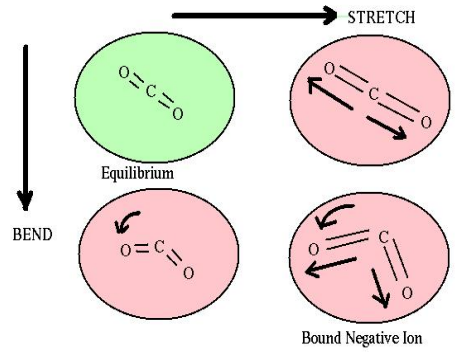
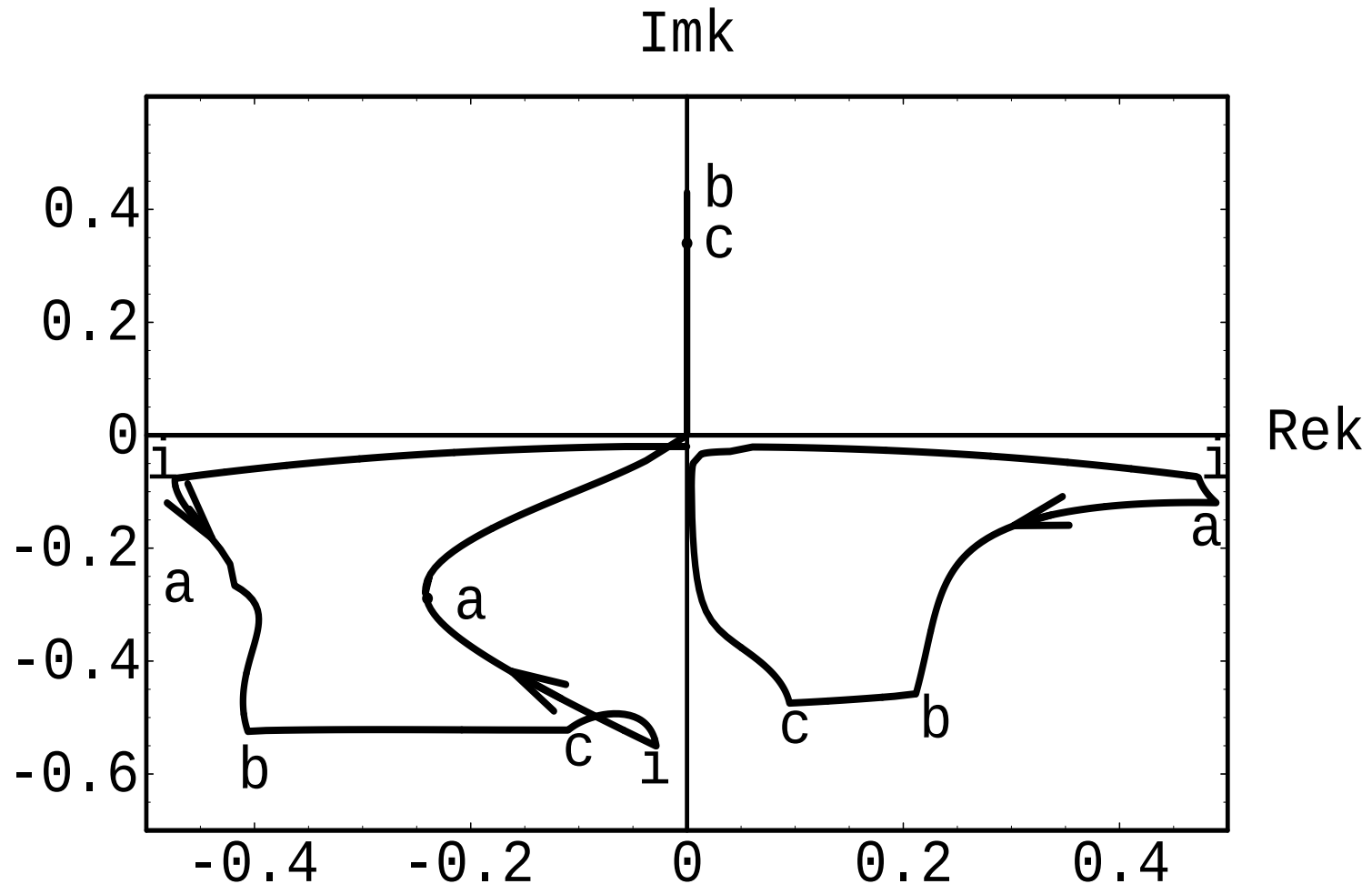


Figure 7: Trajectories of the S-matrix poles as we stretch the molecule


Imk
Rek
0.4
0.2
0
-0.2
-0.4
-0.6
-0.4
-0.2
0
0.2
0.4
b
c
a
i
a
i
a
b
c
c
b
i


STRETCH
BEND
Equilibrium
Bound Negative Ion


Imk
Rek
0.4
0.2
0
-0.2
-0.4
-0.6
-0.4
-0.2
0
0.2
0.4
b
c
1
a
a
b
c
1
1
a
c
b

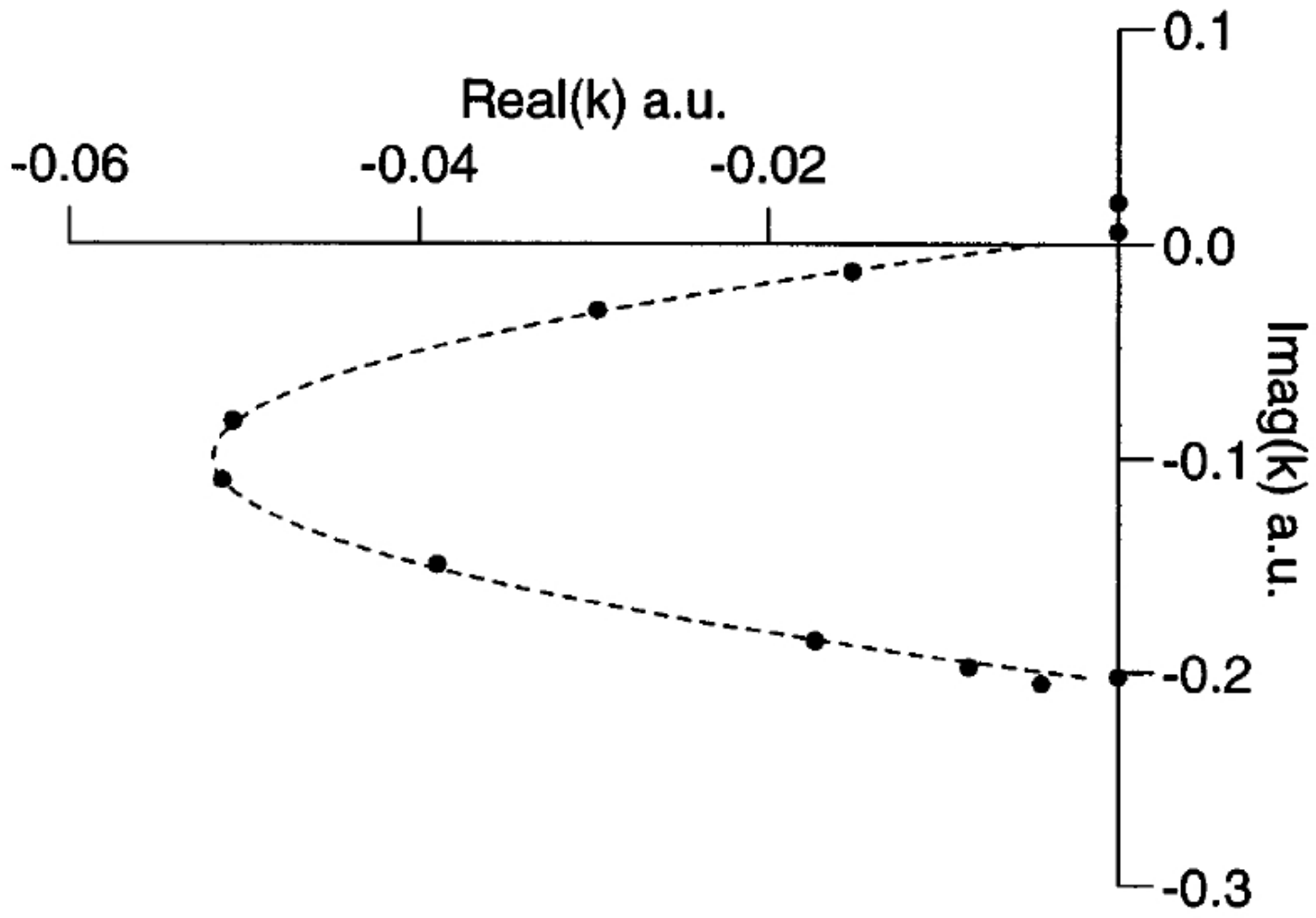


Figure 8: R-matrix siegert calculation for CO_2^- by L. A. Morgan (PRL **80** 1873 (1998))

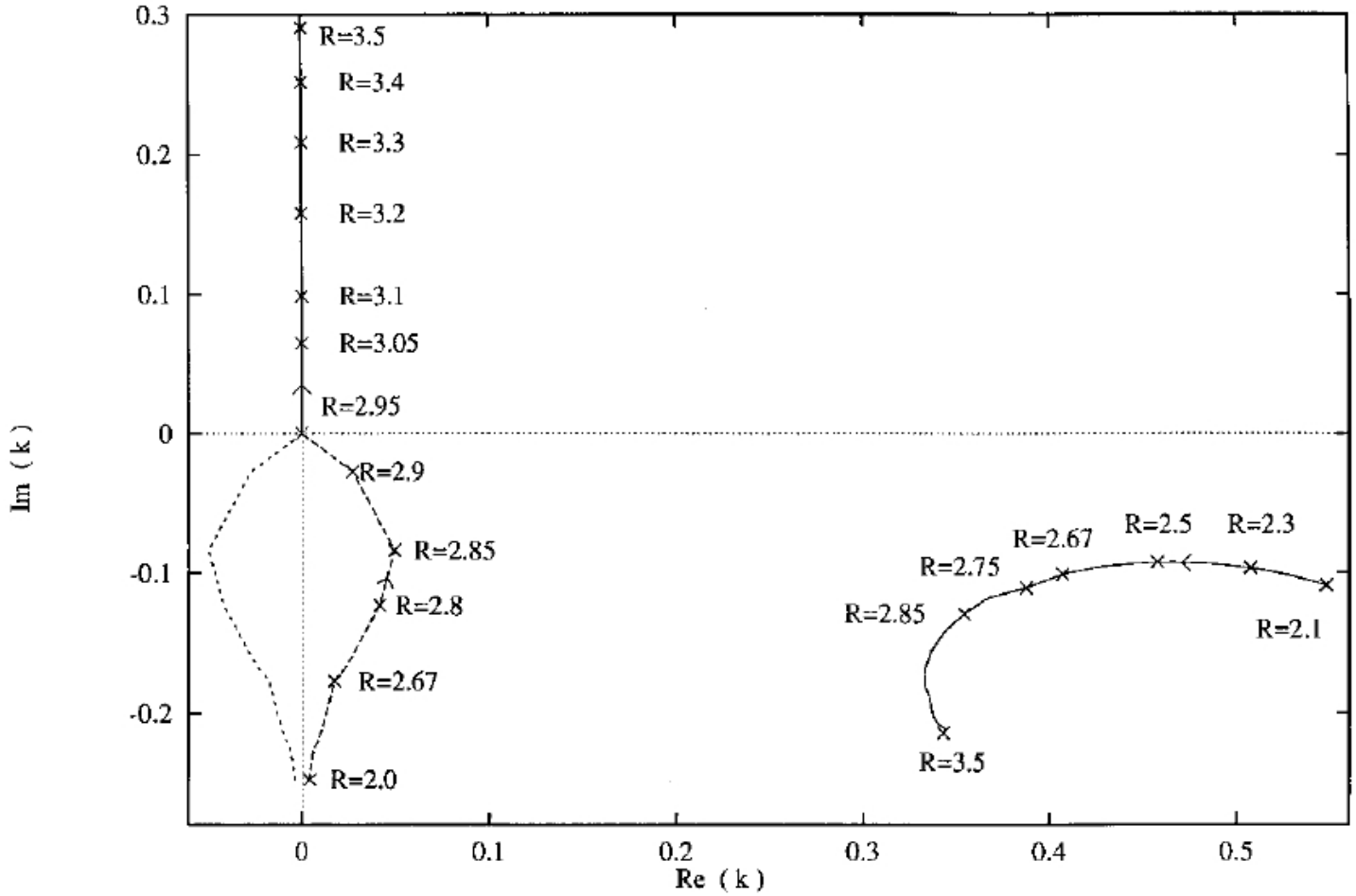


Figure 9: HBr S-matrix poles in the complex k-plane as a function of the stretch. R matrix Siegert calculations by Fandreyer and Burke (J Phys B 29 (1996) 339-343)

Conclusions

- Both the virtual state and the resonance connect with the CO_2^- bound state, depending on the path.

- New physics in the switch from diatomic to polyatomic molecules

  ⋆ Topology for two vibrational degrees of freedom suggests a Berry phase.

More info?

slides → http://www.lbl.gov/CS/amo_theory/

paper → Vanroose, McCurdy and Rescigno, PRA **66** 032720 (2002)